

Theoretical study of bosonic atoms with competing short- and global-range interactions in an optical lattice

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We consider bosonic atoms loaded into optical lattices with cavity-mediated infinite-range interactions. Competing short- and global-range interactions cultivates a rich phase diagram. With a systematic field-theoretical perspective, we present an *analytical* construction of global ground-state phase diagram. We derive an effective theory describing compressible superfluid and supersolid states. We construct a self-consistent mean-field theory and find numerical results consistent with our theoretical analysis.

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Recent experimental realization of competing short- and infinite-range interactions [1] for bosonic atoms in optical lattices has opened a new avenue for exploring new phases of matter. This is achieved by trapping quantum gases in an optical lattice inside a high finesse optical cavity. The infinity-range interactions is mediated by a vacuum mode of the cavity and can be independently controlled by tuning the cavity resonance [2–4]. Essential physics of this system falls into the category of the extended Hubbard model [5], and has been investigated by mean-field theories and quantum monte carlo simulation and various exotic phases have been predicted [6–13].

Ultracold gases in optical lattices are one of the most intriguing systems in which the power of atomic and laser physics can be exploited to explore generic phenomena of solid-state physics [14]. They have been proven to be impressively successful in simulating strongly correlated models like the Bose-Hubbard models, which features a quantum phase transition from a superfluid to a Mott insulating phase [15, 16]. Adding to the excitement is the experimental realization of global-range interactions [1], which raises the fascinating possibility of exploring emergent phenomena such as self-organizing structures. Theoretical understanding of this interesting system is still in its infancy, and this calls for insights from various perspectives. In this work, we shall investigate this problem from a field-theoretical approach [17–23], which allows to treat both compressible and non-compressible phases.

We consider the system described by the following canonical Hamiltonian realized very recently [1]

$$\hat{H} = - \sum_{\langle ij \rangle} (t_{ij} \hat{b}_i^\dagger \hat{b}_j + h.c.) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \frac{K}{M} \left[\sum_{i \in e} \hat{n}_i - \sum_{i \in o} \hat{n}_i \right]^2 - \sum_i \mu \hat{n}_i. \quad (1)$$

Here $\hat{b}_i^\dagger (\hat{b}_i)$ are the bosonic creation (annihilation) operators of an atom at lattice site i , $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the

associated number operator, and M is the total number of lattice sites. The subscript e (o) refers to even (odd) lattice sites $i = (i_x, i_y)$ of square lattice potential defined as $i_x + i_y \in \text{even (odd)}$, and $\langle ij \rangle$ denotes pair of site i and j . The first term represents the kinetic energy resulting from the tunneling between sites with hopping amplitude t_{ij} and supports superfluidity. The second term describes the on-site repulsive interaction with strength $U > 0$. It prefers balanced atom populations on even and odd sites and vanishing spatial coherence. The third term introduces the infinite-range interactions with strength $K > 0$, which favors an overall even-odd imbalance. Interplay of three energy scales is expected to give rise to a multitude of ground-state manifolds. The chemical potential μ is introduced to fix the average particle number N .

Within the framework of Euclidean functional integral, the partition function of the system may be cast as $\mathcal{Z} = \int \mathcal{D}[b_i^*, b_i] e^{-S}$ with the action given by [24, 25] $S = \int_0^\beta d\tau \sum_i [b_i^* \partial_\tau b_i + H(b_i^*, b_i)]$, here $\beta = 1/k_B T$ is the inverse temperature. To decouple the off-site terms in the action, we introduce a real field $\theta(\tau)$ and complex bosonic fields $\Psi_i(\tau)$ by performing Hubbard-Stratonovich transformations, resulting in an equivalent representation of the partition function

$$\mathcal{Z} = \int \mathcal{D}[\Psi_i^*, \Psi_i] \int \mathcal{D}[\theta, b_i^*, b_i] e^{-S_R}, \quad (2)$$

where the resultant action is given by $S_R =$

$\int_0^\beta d\tau \sum_{ij} \Psi_i^* t_{ij}^{-1} \Psi_j + S_0 + S_I$ with

$$S_0 = \int_0^\beta d\tau \left[\frac{K}{M} \theta^2 - 2 \frac{K}{M} \theta \left(\sum_{i \in e} b_i^* b_i - \sum_{i \in o} b_i^* b_i \right) \right] + \sum_i \left[b_i^* (\partial_\tau - \mu) b_i + \frac{U}{2} b_i^* b_i^* b_i b_i \right], \quad (3)$$

$$S_I = - \int_0^\beta d\tau \sum_i (\Psi_i^* b_i + b_i^* \Psi_i). \quad (4)$$

Before embarking on detailed analysis with field-theoretical machinery, we make some comments. The free part S_0 is readily solvable since the corresponding Hamiltonian $\hat{H}_0(\theta) = \sum_i \hat{H}_{0i}(\theta)$ can be diagonalized in the occupation number representation. With the interacting part S_I present, the physics could not be solved in a close form, however, we can gain physical insights by seeking perturbative expansion on top of S_0 in terms of fields Ψ_i , which serves as the superfluid order parameter.

Now we subject the action S_R to a saddle point analysis. Extremum of variation of the action with respect to $\theta(\tau)$ yields $\theta_0 = \sum_{i \in e} b_i^* b_i - \sum_{i \in o} b_i^* b_i$. The physical meaning is clear: θ counts the particle number difference between even sites and odd sites, and θ_0 could be regarded as an order parameter representing charge degrees of freedom. It is easy to notice that quantum fluctuation of θ field only gives a trivial factor to the partition function. Therefore, we are satisfied to replace $\theta(\tau)$ by θ_0 .

Let's consider the atomic limit where the hopping amplitude between sites is negligible ($t_{ij}/U = 0$), and the resultant action reduces to a free one: $S_R = S_0$. The eigenvalue corresponding to \hat{H}_0 for per "supercell" (with one even and one odd sites) after taking account of the self-consistency conditions for θ is given by

$$E(n_e, n_o) = \frac{U}{4} \left[(n_e + n_o) - (1 + \frac{2\mu}{U}) \right]^2 + \frac{U}{4} \left[(1 - \frac{2K}{U})(n_e - n_o)^2 - (1 + \frac{2\mu}{U})^2 \right]. \quad (5)$$

Here $n_e(n_o)$ represents the occupation number of one even (odd) site. The ground state is achieved by minimizing the eigenvalue $E(n_o, n_e)$ with respect to quantum numbers n_e and n_o . Since the system enjoys an Ising-type \mathbb{Z}_2 symmetry corresponding to exchange of even and odd sites, we may choose $n_e \geq n_o$ from now on. To facilitate the analysis, we define $1 + 2\mu/U = n + x$, with $n = \text{int}[1 + 2\mu/U]$ being the integer closest to $1 + 2\mu/U$, and $x \in (-1/2, 1/2)$. Firstly, let's consider the case $K/U \in (0, 1/2)$, the system is in a Mott insulating (MI) phase with $n_e = n_o = n/2$ if n is even. If n is odd, then the system is in the MI phase when $K/U < |x|$, and in a partially polarized charge density wave (CDW) phase with $n_e = n_o + 1 = (n + 1)/2$, vice versa. Secondly,

if $K/U \in (1/2, 1)$, the system enters into a fully polarized CDW phase with $n_e = \text{int} \left[\frac{1+2\mu/U}{2(1-K/U)} \right]$ and $n_o = 0$. Finally, if $K/U > 1$, the ground energy is unbounded from below rendering that the system becomes unstable toward collapse. The above discussions for the ground-state phase diagram are summarized in Fig. 1.

The low temperature properties of the system may be captured by only considering the particle and hole excitations on one supercell [26], since tunneling between sites are completely neglected and hence the system consists of isolate pair sites. For brevity, let us define $C_p = \sum_{s=e,o} e^{-\beta E_{sp}}$ and $C_h = \sum_{s=e,o} e^{-\beta E_{sh}}$, where E_{sp} and E_{sh} is the particle and hole excitation on $s = (e/o)$ site, respectively. To put it explicitly, $E_{ep} = E(n_e + 1, n_o) - E(n_e, n_o)$ and $E_{eh} = E(n_e - 1, n_o) - E(n_e, n_o)$, and similarly for E_{op} and E_{oh} . The partition function on one supercell is therefore approximated as $z_0 = e^{-\beta E(n_e, n_o)} (1 + C_p + C_h)$. The variation of density fluctuations on a supercell is given by $\delta n = (C_p - C_h)/(1 + C_p + C_h)$. Equivalently interesting is the square density fluctuations $\delta n^2 \equiv \langle n^2 \rangle - \langle n \rangle^2$, which is related to the isothermal compressibility via thermodynamic relation $\delta n^2 = \langle n \rangle^2 \kappa_T v_0 / \beta$ with v_0 being the volume of one supercell. We find that $\delta n^2 = (C_p + C_h + 4C_p C_h)/(1 + C_p + C_h)^2$. The temperature dependence of δn and κ_T is shown in Fig. 2. At zero temperature, the particle number fluctuation and thermal compressibility is frozen out, indicating its non-compressible nature. It clearly indicates that the larger K/U is, the larger thermal fluctuation it induces. We attribute this fluctuation-enhancing behavior to the delocalizing effects brought about by the infinite-range interactions.

We proceed to take into account the effects of a finite hopping amplitude. We can evaluate the partition function by performing Taylor expansion in the exponent

$$\frac{\mathcal{Z}}{\mathcal{Z}_0} = \int \mathcal{D}[\Psi_i^*, \Psi_i] e^{-\int d\tau \sum_{ij} \Psi_i^* t_{ij}^{-1} \Psi_j} \left\langle \sum_{l=0} \frac{S_I^l}{l!} \right\rangle_0, \quad (6)$$

where $\langle O \rangle_0 = (\int e^{-S_0} O) / (\int e^{-S_0})$. To the quadratic order in the fields Ψ_i , by transforming to momentum-frequency representation, we obtain $\mathcal{Z}/\mathcal{Z}_0 = \int \mathcal{D}[\Psi^*(k), \Psi(k)] e^{-S_g}$ with the gaussian action given by

$$S_g = \frac{M}{2} \sum_{k=(\mathbf{k}, iw_n)} \Psi^\dagger(k) \mathcal{G}^{-1}(k) \Psi(k), \quad (7)$$

where we have defined $\Psi(k) = (\Psi_e(k), \Psi_o(k))^T$, and used a shorthand notation $k = (\mathbf{k}, iw_n)$, with w_n being the bosonic Matsubara frequencies. The inverse Green's function assumes the form of 2×2 matrix

$$-\mathcal{G}^{-1} = \begin{pmatrix} \frac{n_e+1}{E_{ep}-iw_n} + \frac{n_e}{E_{eh}+iw_n} & -\tilde{t}^{-1}(\mathbf{q}) \\ -\tilde{t}^{-1}(\mathbf{q}) & \frac{n_o+1}{E_{op}-iw_n} + \frac{n_o}{E_{eh}+iw_n} \end{pmatrix} \quad (8)$$

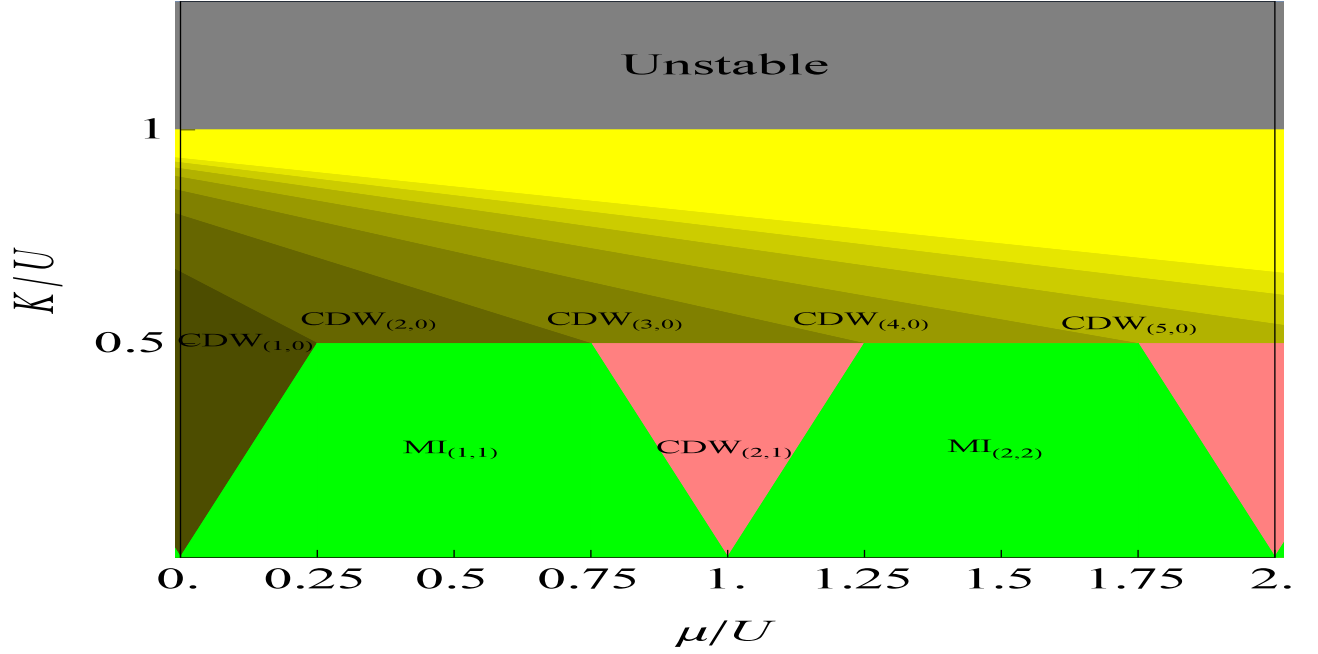


FIG. 1. (color online). Global ground-state phase diagram spanned by μ/U and K/U at atomic limit ($t_{ij}/U = 0$). The phase diagram can be loosely divided into three regimes depending on the strength of infinite-range interaction: (1) $K/U \in (0, 0.5)$, the system is either in a Mott insulating (MI) phase with $n_e = n_o$ or in a partially polarized charge density wave (CDW) phase with $n_e - n_o = 1$, where we always assume $n_e \geq n_o$ as the system enjoys an Ising-type \mathbb{Z}_2 symmetry; (2) $K/U \in (0.5, 1)$, the system is in a fully polarized CDW phase with $n_o = 0$; (3) $K/U > 1$, the system is unstable toward collapse.

In the above, $\tilde{t}^{-1}(\mathbf{q})$ is the Fourier transform of t_{ij}^{-1} . For convenience we shall consider the nearest neighbor hopping only with amplitude t , then $\tilde{t}^{-1}(\mathbf{q}) = 1/[2t \sum_{j=1}^d \cos(k_j \lambda/2)]$, with d being the dimension of the system and λ being the wavelength of the laser field forming the optical lattices.

The excitation spectrum of the system corresponds to the poles of the Green's function. It can be readily found by seeking solutions ω for the secular equations $\det \mathcal{G}^{-1}(\mathbf{k}, \omega) = 0$. It features four branches of excitation spectrum ω_i ($i=1..4$), as shown in Fig. 3 at $k = (\vec{0}, 0)$ in terms of the tuning parameter zt/U with $z = 4$ being the coordination number of square lattices. In absence of hopping ($zt = 0$), the incompressible $MI_{(1,1)}$ phase possesses only one type of particle excitations and one type of hole excitations, while incompressible $CDW_{(2,1)}$ phase carrying charge order possesses two types of particle excitations and two types of hole excitations. At a finite hopping, these two phases both accommodate two branches of particle excitations and two branches of hole excitations. The minimal energy difference between one particle excitation and one hole excitation corresponds to the energy gap for density fluctuations. This excitation gap becomes soft at the phase boundary where phase transition from a non-compressible phase to a compressible phase occurs.

The phase boundary separating the superfluid phase and the non-compressible phase occurs [19, 20, 27] at

$\det \mathcal{G}^{-1}(0, 0) = 0$, which yields

$$\left(\frac{n_e + 1}{E_{ep}} + \frac{n_e}{E_{eh}} \right) \left(\frac{n_o + 1}{E_{op}} + \frac{n_o}{E_{oh}} \right) = \frac{1}{(zt)^2}. \quad (9)$$

We show the phase boundary in Fig. 4. Evidently the regime of MI phase diminishes as K/U increases. In stark contrast, the regime of CDW phase gets broadened as K/U increases. This is caused by the delocalizing effect of infinite-range interaction, favoring the formation of density modulation in the form of a checkerboard pattern with alternating site occupation.

To explore the physics of compressible superfluid and supersolid phases, we proceed even further by evaluating the action to the quartic order in order parameter Ψ_i , $S = S_0 + S_g + S_4$ with $S_4 = \sum_{ss'} \sum_{k+l=m+n} u_{ss'} \Psi_s^*(k) \Psi_{s'}^*(l) \Psi_{s'}(m) \Psi_s(n)$, where we may evaluate the coefficients $u_{ss'}$ on shell. By performing derivative expansion, we keep only the most relevant terms in a long-wavelength approximation, and obtain an effective action of Ginzburg-Landau-Wilson type [28, 29]

$$\begin{aligned} S - S_0 = & \int d\tau \frac{d^2 \mathbf{r}}{2} \sum_s \left(r_s |\Psi_s|^2 + a_s \Psi_s^* \partial_\tau \Psi_s + b_s |\partial_\tau \Psi_s|^2 + u_{ss} |\Psi_s|^4 \right) \\ & + \int d\tau \frac{d^2 \mathbf{r}}{2} \left[r_{eo} \Psi_e^* \left(1 - \frac{\lambda^2 \nabla^2}{16} \right) \Psi_o + c.c + u_{eo} |\Psi_e|^2 |\Psi_o|^2 \right]. \end{aligned} \quad (10)$$

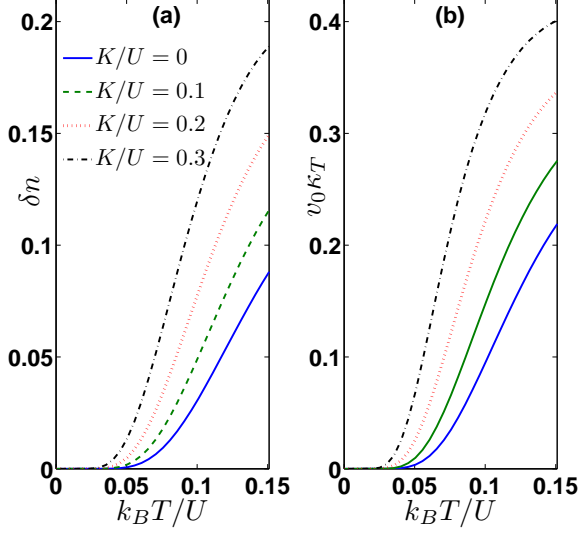


FIG. 2. (color online). Temperature dependence of (a) the variation of particle number δn on one supercell (with one even site and one odd site) and (b) isothermal compressibility κ_T for $MI_{(1,1)}$ phase at different infinite-range interaction strength $K/U = 0, 0.1, 0.2$ and 0.3 . Here $\mu/U = 0.60$, and v_0 is the volume of one supercell.

To present the coefficients above in a succinct fashion, we define $A_s = (n_s + 1)/E_{sp}^2$ and $B_s = n_s/E_{sh}$. Then the relevant coefficients are given as follows: $r_s = -(A_s E_{ps} + B_s E_{hs})$, $a_s = A_s - B_s$, $b_s = A_s/E_{sp} + B_s/E_{sh}$, $r_{eo} = 1/(zt)$, $u_{ss} = (A_s + B_s)(A_s E_{sp} + B_s E_{sh}) - A_s(n_s + 2)/E_{s2p} - B_s(n_s - 1)/E_{s2h}$, and

$$\frac{U_{eo}}{K} = A_e A_o \frac{E_{ep} + E_{op}}{E_{ep} + E_{op} + K} + B_e B_o \frac{E_{eh} + E_{oh}}{E_{eh} + E_{oh} + K} - \sum_{s=e,o} A_s B_{-s} \frac{E_{sp} + E_{-sh}}{E_{sp} + E_{-sh} - K}. \quad (11)$$

Here $E_{e2p} = E(n_e + 2, n_o) - E(n_e, n_o)$ is the “double particles” excitation energy at even sites and $E_{e2h} = E(n_e - 2, n_o) - E(n_e, n_o)$ is the “double holes” excitation energy at even sites, and similar expressions for E_{o2p} and E_{o2h} . The universality class and associated quantum criticality is intimately related to the relevant parameters given above.

At low energy, we seek field configurations that are spatially and temporally homogenous. The grand potential $\Omega = -\ln \mathcal{Z}/\beta$ of the system reduces to a simple form as follows

$$\Omega = \Omega_0 + \sum_{s=e,o} r_s |\Psi_s|^2 + r_{eo} (\Psi_e^* \Psi_o + c.c.) + \sum_{s=e,o} u_{ss} |\Psi_s|^4 + u_{eo} |\Psi_o|^2 |\Psi_e|^2. \quad (12)$$

We notice that $r_{eo} > 0$, so Ψ_e and Ψ_o is out of phase, and we may choose both of them to be real. Quite gen-

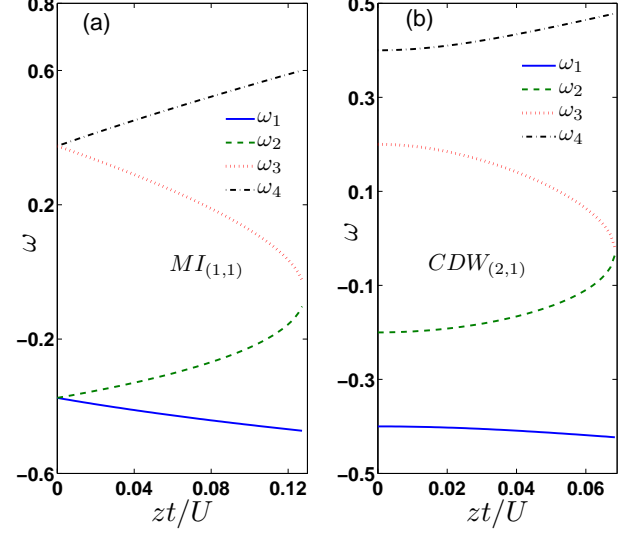


FIG. 3. (color online). Four branches of excitation spectrum ω_i ($i=1..4$) at momentum $\mathbf{k} = (\vec{0}, 0)$ as a function of tunneling parameter zt/U for (a) the $MI_{(1,1)}$ phase with $\mu/U = 0.50$ and $K/U = 0.25$; (b) the $CDW_{(2,1)}$ phase with $\mu/U = 1.0$ and $K/U = 0.40$. The upper two branches are particle excitations and the lower two branches are hole excitations. For both insulating phases, there exists an energy gap for a particle-hole excitation, manifesting their non-compressible nature. Here $z = 4$ is the coordination number for square lattices.

erally, the realization of the phase is determined by seeking the global minimum of Ω . The saddle point condition $\partial\Omega/\partial\Psi_s = 0$ yields $2r_s\Psi_s + 2r_{eo}\Psi_{-s} + 4u_{ss}\Psi_s^3 + 2u_{eo}\Psi_s\Psi_{-s}^2 = 0$. Clearly, if $\Psi_s = 0$, then from the above equation we immediately obtain $\Psi_{-s} = 0$, namely Ψ_e and Ψ_o vanishes identically at the transition point. The phase boundary is determined by $r_o r_e = r_{eo}^2$, which reproduces Eq. (9). Typically close to the phase boundary, the order parameter field satisfies a simple scaling $\Psi_s/\Psi_{-s} = -r_{eo}/r_s = -\sqrt{r_{-s}/r_s}$. At this level the phase transition is of a continuous one. However, when the system is deep into a superfluid phase with a crystalline order, there may induce a structural transition (where quantum numbers n_e and n_o change) from a supersolid (SS) phase to a superfluid (SF) phase, typically a first-order one, since it involves a discontinuous change of the free energy. In broken-symmetry phases, the order parameters are determined by the coefficients. The grand potential is fully determined as $\Omega = \Omega_0(n_e, n_o, \mu) + \delta\Omega(n_e, n_o, \mu, zt)$. Given μ and zt , the global minimum of the grand potential is achieved by minimizing over non-negative integer of n_e and n_o . However, it should be noted that such perturbative treatment only give qualitatively sensible physics for the regime deep into the compressible phase.

Self-consistent mean-field theory. The mean-field Hamiltonian for a supercell can be constructed as fol-

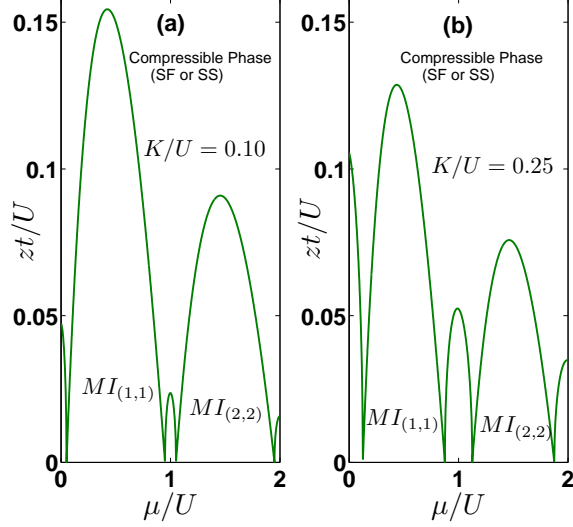


FIG. 4. (color online). The phase boundary separating compressible (SF or SS) and non-compressible phases (MI or CDW) for two typical infinite-range interaction strengths: (a) $K/U = 0.10$ and (b) $K/U = 0.25$. Increasing K/U leads to the broadening of the region of *CDW* phases and the shrinking of the region of *MI* phases. Here a SF phase stands for a superfluid phase which has off-diagonal long-range order, and a SS phase stands for a supersolid phase which has both diagonal and off-diagonal long-range orders.

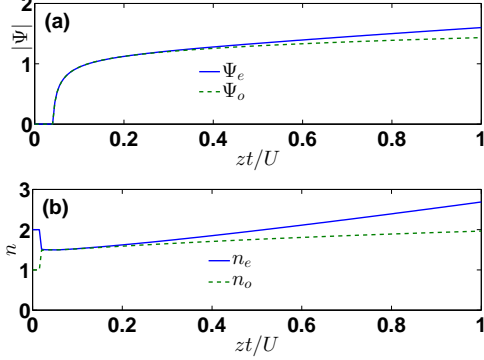


FIG. 5. (color online). (a) The magnitude of the order parameters $|\Psi_e|$ and $|\Psi_o|$ in the supersolid phase as a function of zt/U ; (b) The density at even site n_e and odd site n_o as a function of zt/U . Here the parameters used here are $\mu/U = 0.98$ and $K/U = 0.45$.

lows:

$$\hat{H}^{MF} = \sum_{s=e,o} \left[\frac{U}{2} \hat{n}_s (\hat{n}_s - 1) - \mu n_s \right] - \frac{K}{2} (n_e - n_o)^2 - zt \left[(\Psi_o \hat{b}_e^\dagger + \Psi_e^* \hat{b}_o - \Psi_o \Psi_e^*) + h.c. \right]. \quad (13)$$

We may diagonalize H^{MF} in the basis spanned by $|n_e\rangle \otimes |n_o\rangle$ by simultaneously imposing self-consistency

conditions $\Psi_e = \langle \hat{b}_e \rangle$ and $\Psi_o = \langle \hat{b}_o \rangle$. The numerical results from this self-consistent theory are shown in Fig. 5, which confirms our field-theoretical analysis carried out previously.

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